AMENDMENTS TO THE CLAIMS

The following listing of claims will replace all prior versions and listings of claims in the application.

LISTING OF CLAIMS

1. (Currently Amended) A computer based method for generating a three-dimensional quantitative structure-activity relationship ~~method~~ of a chemical compound, the compound derived from a plurality of molecules each having a related pharmacological activity and ~~for determining and~~ visually displaying a region of the compound in which altering one or more physiochemical characteristics of [[a]] said region ~~compound which modulates a~~ can predict a change to said pharmacological activity of said compound, the method comprising:

a process A of superposing a three-dimensional spatial arrangement of atoms of [[a]] said plurality of molecules using Cartesian three-dimensional x, y, and z atomic coordinates in a virtual space;

a process B of performing cluster analysis of the atomic coordinates of said atoms of said plural molecules thus superposed in said virtual space and thereby generating represented points;

a process C of calculating interactions selected from the group consisting of steric interactions, electrostatic interactions, hydrophobic interactions and combinations thereof between the atoms of said plural molecules thus superposed and said represented points using an evaluation function or indicator variables;

a process D of statistically analyzing said interactions using regression analysis to generate a plurality of correlation components between said calculated interactions

and ~~a known~~ said pharmacological activity of ~~one of~~ said molecules and forming an activity prediction formula; and

a process E of assigning an activity prediction value to each atom of said plurality of molecules and displaying said activity prediction values overlayed on a region of said compound on a graphical display,

wherein said process B of cluster analysis further comprises:

a first process B1 of calculating the coordinates of the atoms contained in said plural molecules thus superposed in said virtual space;

a second process B2 of calculating interatomic distances between each atom and other atoms superposed and identifying the shortest interatomic distance among thus calculated interatomic distances and two atoms constituting the shortest interatomic distance;

a third process B3 of deleting said two atoms having the shortest interatomic distance from said three-dimensional space and generating an atom which represents said two atoms in the weighted average coordinates of said two atoms to delete, when the shortest interatomic distance thus calculated is equal to or smaller than a predetermined threshold value;

a fourth process B4 of returning to said second process B2 after said third process B3 and executing said second process B2 including said atoms formed during said third process B3; and

a fifth process B5 of terminating said process B when the shortest interatomic distance thus calculated is exceeds said predetermined threshold.

2. (Cancelled)

3. (Cancelled)

4. (Currently Amended) A computer program product for determining a three-dimensional quantitative structure-activity relationship ~~method for determining and~~ of a compound, the compound derived from a plurality of molecules each having a related pharmacological activity and visually displaying a region of the compound in which altering one or more physicochemical characteristics of [[a]]said region ~~compound~~ can predict a change to said ~~which which modulates a~~ pharmacological activity of said compound, said computer program ~~making a computer execute~~product comprising computer executable instructions embodied in a computer memory for performing steps comprising:

a process A of superposing a three-dimensional spatial arrangement of atoms of [[a]] said plurality of molecules using Cartesian three-dimensional x, y, and z atomic coordinates in a virtual space;

a process B of performing cluster analysis of the atomic coordinates of said plural molecules thus superposed in said virtual space and thereby generating represented points;

a process C of calculating interactions selected from the group consisting of steric interactions, electrostatic interactions, hydrophobic interactions and combinations thereof between the atoms of said plural molecules thus superposed and said represented points using an evaluation function or indicator variables;

a process D of statistically analyzing said interactions using regression analysis to generate a plurality of correlation components between said calculated interactions and ~~a known~~ said pharmacological activity of ~~one of~~ said molecules and forming an activity prediction formula; and

a process E of assigning an activity prediction value to each atom of said plurality of molecules and displaying said activity prediction value overlayed on said compound on a graphical display,

wherein said process B of cluster analysis further comprises:

a first process B1 of calculating the coordinates of the atoms contained in said plural molecules thus superposed in said virtual space;

a second process B2 of calculating interatomic distances between each atom and other atoms superposed and identifying the shortest interatomic distance among thus calculated interatomic distances and two atoms constituting the shortest interatomic distance;

a third process B3 of deleting said two atoms having the shortest interatomic distance from said three-dimensional space and generating an atom which represents said two atoms in the weighted average coordinates of said two atoms to delete, when the shortest interatomic distance thus calculated is equal to or smaller than a predetermined threshold value;

a fourth process B4 of returning to said second process B2 after said third process B3 and executing said second process B2 including said atoms formed during said third process B3; and

a fifth process B5 of terminating said process B when the shortest interatomic distance thus calculated is exceeds said predetermined threshold.

5. (Cancelled)

6. (Cancelled)

7. (Currently Amended) The method according to Claim 1, wherein the process C of calculating interactions includes an evaluation ~~formula~~ function selected from the group consisting of rapid molecular ~~superstition~~superposition, seal-type, indicated variables and combinations thereof.

8. (Currently Amended) The method according to Claim 4, wherein the process C of calculating interactions includes an evaluation ~~formula~~ function selected from the group consisting of rapid molecular superstition, seal-type, indicated variables and combinations thereof.

9. (New) A computer based method for designing a test compound which will bind to a biologically active protein, said biologically active protein is known to bind to a plurality of molecules having related pharmacological activities with said biologically active protein, said method comprising:

a process A of superposing a three-dimensional spatial arrangement of atoms of a plurality of molecules using Cartesian three-dimensional x, y, and z atomic coordinates in a virtual space;

a process B of performing cluster analysis of the atomic coordinates of said atoms of said plural molecules thus superposed in said virtual space and thereby generating represented points;

a process C of calculating interactions selected from the group consisting of steric interactions, electrostatic interactions, hydrophobic interactions and combinations thereof between the atoms of said plural molecules thus superposed and said represented points using an evaluation function or indicator variables;

a process D of statistically analyzing said interactions using regression analysis to generate a plurality of correlation components between said calculated interactions and said related pharmacological activity of one of said molecules and forming an activity prediction formula;

a process E of assigning an activity prediction value to each atom of said plurality of molecules and displaying said activity prediction value overlayed on said compound on a graphical display, and

a process F of synthesizing a test compound with atoms arranged in a molecular conformation having one or more regions determined to enhance said pharmacological activity of said test compound with said biologically active protein;

wherein said process B of cluster analysis further comprises:

a first process B1 of calculating the coordinates of the atoms contained in said plural molecules thus superposed in said virtual space;

a second process B2 of calculating interatomic distances between each atom and other atoms superposed and identifying the shortest interatomic distance among thus calculated interatomic distances and two atoms constituting the shortest interatomic distance;

a third process B3 of deleting said two atoms having the shortest interatomic distance from said three-dimensional space and generating an atom which represents said two atoms in the weighted average coordinates of said two atoms to delete, when the shortest interatomic distance thus calculated is equal to or smaller than a predetermined threshold value;

a fourth process B4 of returning to said second process B2 after said third process B3 and executing said second process B2 including said atoms formed during said third process B3; and a fifth process B5 of terminating said process B when the shortest interatomic distance thus calculated is exceeds said predetermined threshold.